

Claims

1. A method of generating an isosteric structure of a polypeptide at least partially containing D-amino acids from 3D-coordinates and sequence information of an L-configurated precursor having an N-terminal amino group or substituted amino group, a C-terminal carboxy group or a carboxy derivative, a backbone and L-amino acid side chains, and comprising the steps of
 - at least partially replacing backbone CO groups with NH groups and vice versa,
 - while keeping fixed the 3D-coordinates of the precursors L-amino acid side chains, the N-terminal amino group or substituted amino group and the C-terminal carboxy group or carboxy derivative.
2. The method according to claim 1 comprising the steps of
 - at least partially replacing backbone CO groups with NH groups and vice versa,
 - while keeping the 3D-coordinates of the precursor's L-amino acid side chains fixed, and replacing the N-terminal amino group or substituted amino group by a carboxy group or carboxy derivative and/or replacing the C-terminal carboxy group or carboxy derivative by an amino group or substituted amino group.
3. The method according to claims 1-2 wherein all backbone CO groups of the precursor are replaced by NH groups and vice versa.
4. The method according to claims 1-3, characterized by
 - at least partially replacing the proline residues or proline residues and their adjacent neighbouring residue in the structure and sequence of the precursor by organic molecules as building blocks mimicking the conformational properties of proline or of proline and its immediately neighbouring residue in the newly configured backbone.
5. The method according to claims 1 to 4 comprising the steps according to figure 1.

6. The method according to claims 1-5 conducted on a computer device.

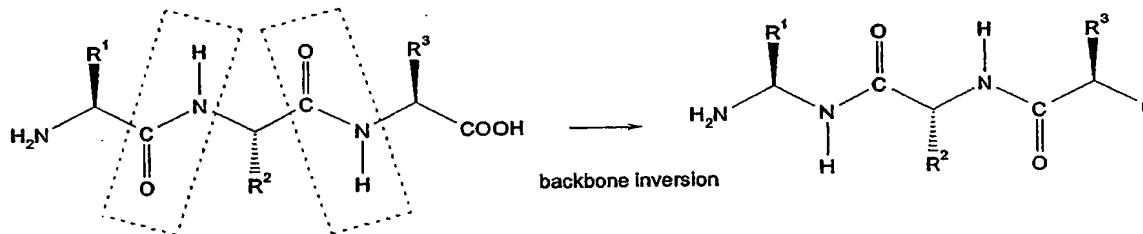
7. A method of generating a polypeptide comprising at least one D-amino acid and/or artificial amino acid, the method comprising the steps of obtaining an isosteric structure by a method of any of claims 1 to 6 and synthesizing the polypeptide of said isosteric structure.

5 8. The method of claim 7 or 8, wherein the polypeptide consists of D-amino acids and/or artificial amino acids.

9. A polypeptide obtainable by a method according to claims 1-8.

10. The polypeptide according to claim 9 having less than 100 residues, in particular 60 or less, or 40 or less residues but at least 7 residues.

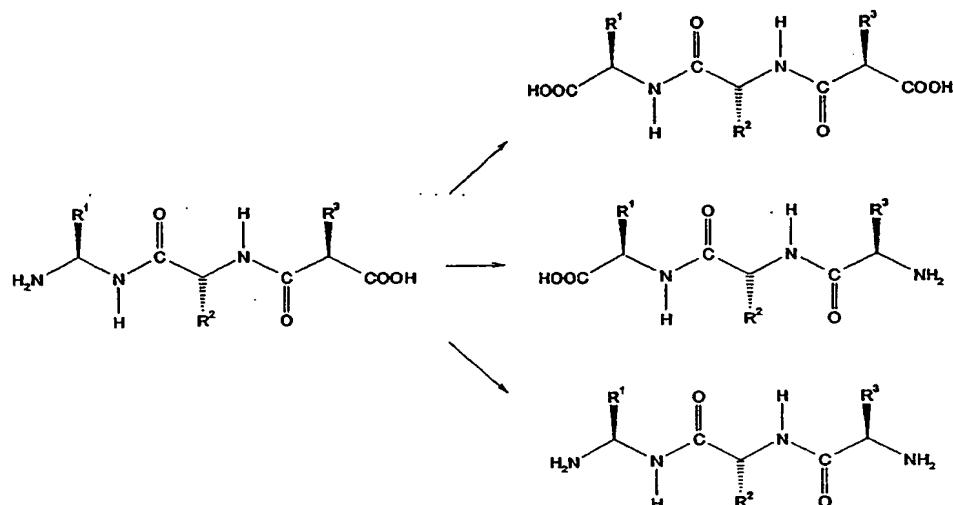
11. The polypeptide according to claims 9-10 being characterized by the replacement of backbone CO with NH groups and vice versa, while C-terminal carboxy and N-terminal amino function are not changed, as illustrated and exemplified non-exclusively in Formula 1:



15 12. The polypeptide according to claim 9-11, in which either the terminal amino group is replaced by a Carboxy-group and/or the terminal carboxy group is replaced by an amino-group or in which N- and C- terminus are exchanged with each other as illustrated and exemplified

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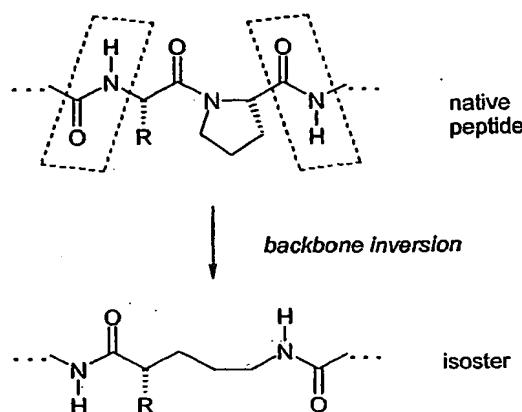
non-exclusively in Formula 2:



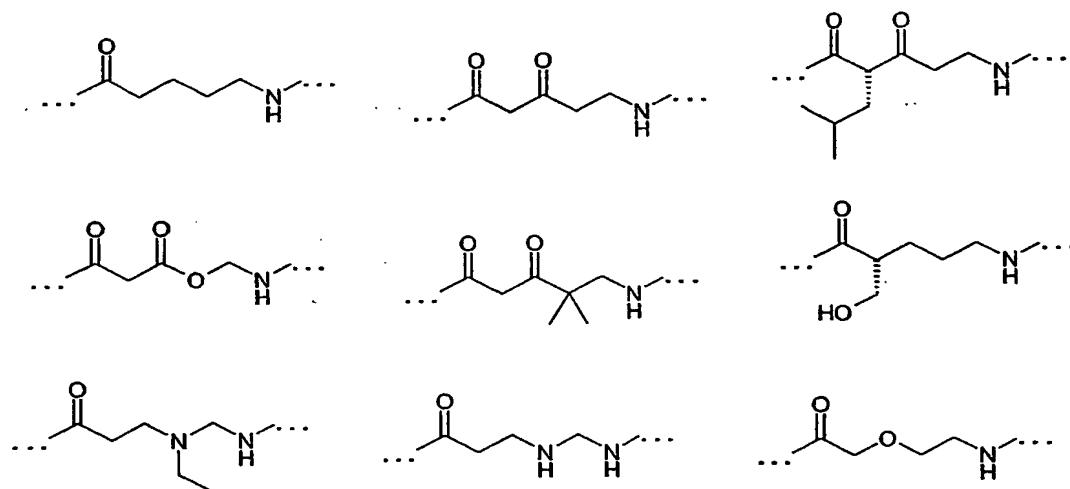
13. The polypeptide according to claims 9-12, wherein at least one proline residue of the precursor is replaced by glycine.

5 14. The polypeptide according to claims 9-13, in which 5-aminovaleric acid and its derivatives described by the generic formula ...-(CO)-X¹-X²-X³-X⁴-NH-..., wherein X¹, X², X³, and X⁴ are independently selected from CH₂, (C=O), NH, NR, O, (CHR), or (CR₂), and wherein R is an amino group, an alcohol, halogen or any organic residue are used to replace a proline residue and its adjacent neighbouring residue in the precursor sequence, as non-exclusively illustrated by Formulas 4, demonstrating the use of 5-aminovaleric acid as building block, and 5, showing the use of exemplary, non-exclusive derivatives of 5-aminovaleric acid as building blocks.

10 15. Formula 4:



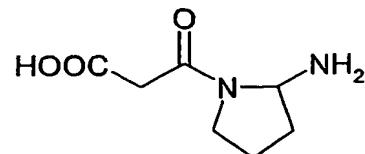
Formula 5:



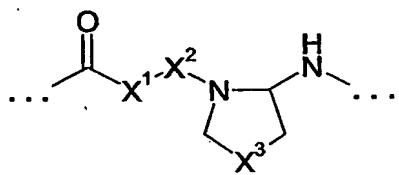
15. A compound having the Formula 7, in particular 3-(2S-Allyloxycarbonyl-amino-pyrrolidin-1-yl)-3-oxo-propionic acid (Formula 6) wherein X^1 , X^2 and X^3 are independently selected from CH_2 , $(\text{C}=\text{O})$, O , S , NH , NR , (CHR) , or (CR_2) , and wherein R is an amino group, an alcohol, halogen or any organic residue; molecules described by the generic formula are non-exclusively illustrated in Formula 8.

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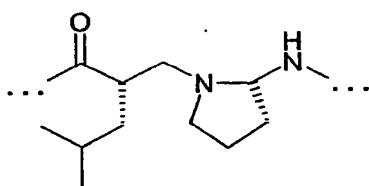
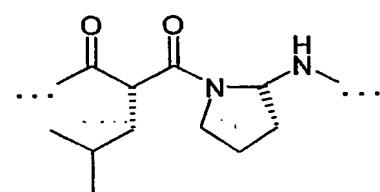
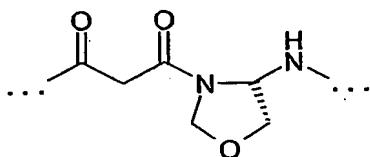
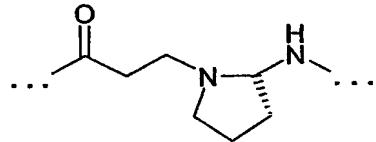
Formula 6:



10 Formula 7:



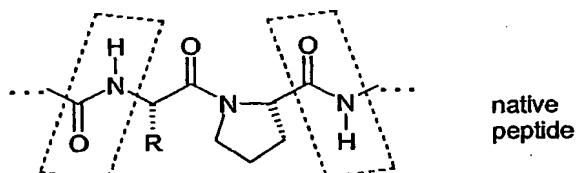
Formula 8:



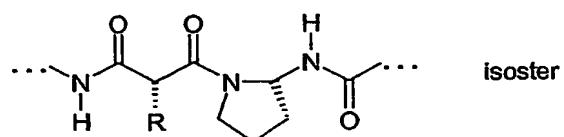
16. The polypeptide according to claims 9-15, in which a building block according to claim 15 is used to replace at least one proline residue and its immediately neighbouring residue as illustrated non-exclusively in

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Formula 9:



↓
backbone inversion

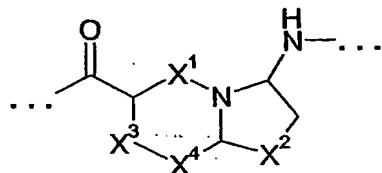


17. A compound of Formula 10, wherein X^1 , X^2 , X^3 and X^4 are independently selected from CH_2 , $(C=O)$, O , S , NH , NR , (CHR) , or (CR_2) , and wherein R is an amino group, an alcohol, halogen or any organic residue, whereby examples of respective molecules are non-exclusively shown in

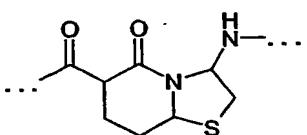
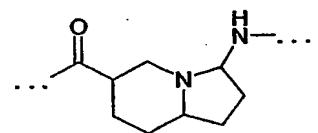
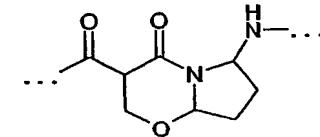
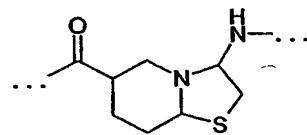
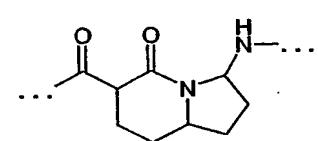
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Formula 11.

Formula 10



Formula 11



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18. The polypeptide according to claims 9-14, 16, in which a building block according to claim 15 is used to replace at least one proline residue and its immediately neighbouring residue.

19. The polypeptide obtainable by claim 9 and using at least one or a free combination of the building blocks specified in claims 12-16 as substitute for a proline or for a proline and its immediately neighbouring residue.

20. The polypeptide according to claims 9-19, modified by acetylation of the N-terminus or amidation of the C-terminus or by acetylation of the N-terminus and amidation of the C-terminus.

21. The polypeptide according to claims 9-20, modified by extension of the precursor sequence by non-binding amino acids at either the C-terminus or at the N-terminus or at both termini, whereby the number of residues added in total is 15 or less, in the preferred case 6 or less.

22. The polypeptide according to claims 9-20, in which one or more amino acid residues other than proline are substituted by conservative exchange using physicochemically related natural or unnatural amino

acid residues, while the binding behaviour and structure required for binding are maintained.

23. A polypeptide comprising at least one D-amino acid and/or artificial amino acid and 5-aminovaleric acid.

5 24. A polypeptide of claim 23, comprising a sequence of a D-amino acid followed by 5-aminovaleric acid followed by a D-amino acid.

25. A polypeptide of claim 23 or 24 consisting of D-amino acids and/or artificial amino acids and at least one 5-aminovaleric acid.

10 26. A polypeptide of any of claims 23 to 25, wherein the 5-aminovaleric acid is substituted by a building block of any one of claims 14, 15 and/or 16.

27. A polypeptide of the amino acid sequence:

ynnignlimqldlllhelqlqtkkts

28. Use of compounds according to claims 9-22 for vaccination or for diagnostic, pharmaceutical or cosmetic purposes.

15 29. Pharmaceutical preparations comprising a compound according to claims 9-22.